

# Statistical properties of the estimator using covariance matrix

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## Abstract

The statistical properties of estimator using covariance matrix for the account of point-to-point correlations due to systematic errors are analyzed. It is shown that the covariance matrix estimator (CME) is consistent for the realistic cases (when systematic errors on the fitted parameters are not extremely large comparing with the statistical ones) and its dispersion is always smaller, than the dispersion of the simplified  $\chi^2$  estimator applied to the correlated data. The CME bias is negligible for the realistic cases if the covariance matrix is calculated during the fit iteratively using the parameter estimator itself. Analytical formula for the covariance matrix inversion allows to perform fast and precise calculations even for very large data sets. All this allows for efficient use of the CME in the global fits.

# INTRODUCTION

Modern particle physics development becomes more and more based on the analysis of precise experimental data. This demands refining of all stages of the data inference including the account of correlations due to systematic uncertainties which are often comparable or even larger than the statistical ones. In particular this problem is important for the precise tests of Standard Model and determination of the parton distributions [1, 2]. Many authors for the sake of simplicity very often use approaches which ignore point-to-point correlations due to systematic errors, i.e. sum all errors in quadrature or drop systematics at all. It is evident that if the systematic errors are important source of the data uncertainty such approaches can lead to the distortion of the estimated errors on the fitted parameters. At the same time the construction of estimators accounting for the correlations is not straightforward since the competitive probabilistic model of data can be used in the analysis. Essentially two generic models are possible: One based on the frequentist treatment of systematic shifts and another one based on the Bayesian approach. This paper is concentrated on the analysis of statistical properties of the estimators within the Bayesian treatment of systematic errors. An introduction into this scope given in Ref. [3] contains argumentation in favor of this approach. The only point that we would like in particular underline here is that the Bayesian treatment is the only constructive way in the case of many sources of systematics when classical treatment which implies introduction of additional parameter for every source of systematic errors can cause great problem with the interpretation/representation of the function of the large number of arguments.

The natural way to account for point-to-point correlations due to systematic errors within Bayesian approach is to use covariance matrix associated with systematic errors (see e.g. Refs. [4, 5]). Meanwhile, there are concerns that the covariance matrix estimator (CME) can result in biased values of the parameters values and their dispersions (see Refs. [6, 7, 8, 9]). In this connection it worth to recall that the estimators accounting for the data correlations often exhibit poor statistical properties regardless they use covariance matrix or not. For example as it was shown in Ref. [10] the sample dispersion estimated from the the correlated Monte Carlo data sets can acquire the bias equal to the dispersion value itself<sup>1</sup>. At the same time the estimators would be unbiased if the covariance matrix is not evaluated from the measurements itself. Indeed, the unbiased estimator for the correlated Monte-Carlo data was constructed in Ref. [11] using the modeled covariance matrix.

Running this way, one can hope to construct the unbiased estimators accounting for systematic errors through covariance matrix, but to be aware of its unbiasedness the study of their properties is needed. In view of lack of the comprehensive information on this scope in literature, this paper is devoted to the analysis of the statistical properties of such estimators with a particular attention paid on the control of the bias. Through the paper the CME properties are compared with the properties of the simplest  $\chi^2$  estimator (SCE) as well as it was done earlier in Ref. [12].

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<sup>1</sup>This effect is connected with the well known fact that the sample dispersion gives biased estimation of the studied distribution dispersion; the correlations merely amplify this bias.

# 1 THE SIMPLEST $\chi^2$ ESTIMATOR

To illustrate our method of the statistical properties analysis we start from the analysis of uncorrelated measurements. In this case, if the data sample  $\{y_i\}$  is supposed to be explicitly described by a theoretical model  $t_i = f_i(\theta^0)$ ,

$$y_i = t_i + \mu_i \sigma_i, \quad (1)$$

where  $\mu_i$  are independent random variables,  $\sigma_i$  are statistical errors,  $i = 1 \dots N$ ,  $N$  is the total number of points in the sample. We adopt that theoretical model parameter  $\theta^0$  is scalar, the generalization of the formula on the case of vector parameter is evident. If  $y_i$  are obtained in the counting experiment with the large number of events,  $\mu_i$  are Gaussian distributed, although it is not crucial for our consideration. As a rule the values of  $\sigma_i$  given in the experimental publications, are the estimators of the  $y_i$  standard deviations, i.e. are random variables, but we neglect their fluctuations. The SCE is based on the minimization of functional

$$\chi^2(\theta) = \sum_{i=1}^N \frac{(f_i(\theta) - y_i)^2}{\sigma_i^2} \quad (2)$$

or, equivalently, solution of the equation

$$\xi(\theta) \equiv \frac{1}{2} \frac{\partial \chi^2}{\partial \theta} = 0. \quad (3)$$

The solution  $\hat{\theta}$  is the estimator of parameter  $\theta$ , which is the random variable depending on  $\{y_i\}$ . To investigate statistical properties of  $\hat{\theta}$  we expand the function  $\xi(\theta)$  around  $\theta^0$  and then apply Legendre inversion to obtain the series for  $\hat{\theta}$  (see Ref. [13] for the details of method). Introducing

$$\begin{aligned} X &= \xi(\theta^0), & a &= - \left\langle \frac{\partial \xi(\theta^0)}{\partial \theta} \right\rangle, \\ b &= \left\langle \frac{\partial^2 \xi(\theta^0)}{\partial \theta^2} \right\rangle, & Y &= \frac{\partial \xi(\theta^0)}{\partial \theta} - \left\langle \frac{\partial \xi(\theta^0)}{\partial \theta} \right\rangle, \end{aligned}$$

one can obtain

$$\hat{\theta} - \theta^0 = \frac{X}{a} + \frac{XY}{a^2} + \frac{bX^2}{2a^3} + \dots \quad (4)$$

where  $\langle \dots \rangle$  means averaging over the samples and the rejected part of the expansion contains the terms with the higher powers of  $1/a$  and/or  $X$  and  $Y$ . In this approximation the dispersion of  $\hat{\theta}$  is

$$D(\hat{\theta}) = \frac{\langle X^2 \rangle}{a^2}$$

and the bias is

$$B(\hat{\theta}) = \frac{\langle X \rangle}{a} + \frac{\langle XY \rangle}{a^2} + \frac{b \langle X^2 \rangle}{2a^3}.$$

For the SCE applied to the sample (1) one can easily obtain

$$\langle X \rangle = 0,$$

$$\langle X^2 \rangle = -a = \sum_{i=1}^N \frac{[f'_i(\theta_0)]^2}{\sigma_i^2},$$

$$\langle XY \rangle = \frac{b}{3} = \sum_{i=1}^N \frac{f'_i(\theta_0) f''_i(\theta_0)}{\sigma_i^2}, \quad (5)$$

where  $f'_i(\theta)$  is the derivative on  $\theta$ . The dispersion and the bias of this estimator are

$$D_0^U(\hat{\theta}) = -\frac{1}{a}, \quad B_0^U(\hat{\theta}) = -\frac{b}{6a^2}. \quad (6)$$

If  $f_i(\theta)$  are the linear functions of  $\theta$  the series (4) is truncated and equation (3) can be solved exactly. One can see that in this case the estimator bias vanishes. For a non-linear data model the expansion (4) contains an infinite number of terms, but the contributions from the highest terms are proportional to the powers of  $D(\hat{\theta})$  and/or to the central moments of  $y_i$  higher than the second. These contributions are progressively suppressed comparing with the main terms if the data statistics rises. Here and through the paper we neglect the contribution from the high moments of  $y_i$ . Remind that the same approximation is used in deducing of the central limit theorem of statistics. This approach can be also used to justify the analysis of a nonlinear data model: The above formula can be applied to the data model with a “weak nonlinearity”, i.e. if its nonlinearity is not significant on the scale of the parameter standard deviation.

Now let the sample to have a common additive systematic error. In accordance with the Bayesian approach to the treatment of systematic errors the measured values are given by

$$y_i = t_i + \mu_i \sigma_i + \lambda s_i, \quad (7)$$

where  $s_i$  are systematic shifts for every point and  $\lambda$  is the random variable with zero average and unity dispersion<sup>2</sup>. Consider the case of one source of systematic error, generalization on the many sources case is straightforward. For the sample (7) we loose statistical independence of measurements and with the account of the their correlations the relevant expression for the dispersion and bias are more complicated

$$\begin{aligned} \langle X^2 \rangle &= \sum_{i,j=1}^N \frac{C_{ij}}{\sigma_i^2 \sigma_j^2} f'_i(\theta_0) f'_j(\theta_0) = -a + \left[ \sum_{i=1}^N \frac{s_i}{\sigma_i^2} f'_i(\theta_0) \right]^2, \\ \langle XY \rangle &= \sum_{i,j=1}^N \frac{C_{ij}}{\sigma_i^2 \sigma_j^2} f'_i(\theta_0) f''_j(\theta_0) \\ &= \frac{b}{3} + \left[ \sum_{i=1}^N \frac{s_i}{\sigma_i^2} f'_i(\theta_0) \right] \left[ \sum_{i=1}^N \frac{s_i}{\sigma_i^2} f''_i(\theta_0) \right], \end{aligned}$$

where  $a$  and  $b$  are given by Eqn. (5),  $C_{ij}$  is the covariance matrix for  $\{y_i\}$

$$C_{ij} = s_i s_j + \delta_{ij} \sigma_i \sigma_j, \quad (8)$$

and  $\delta_{ij}$  is Kronecker symbol. Expressions for  $a$  and  $b$  are the same as for the uncorrelated data case. In terms of the  $N$ -component vectors

$$\rho_i = \frac{s_i}{\sigma_i}, \quad \phi_1^i = \frac{f'_i(\theta_0)}{\sigma_i}, \quad \phi_2^i = \frac{f''_i(\theta_0)}{\sigma_i}$$

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<sup>2</sup>Emphasize, that  $\lambda$  is not necessary Gaussian distributed.

the dispersion and the bias in this case can be expressed as

$$D_0^A(\hat{\theta}) = \frac{1}{\phi_1^2} (1 + \rho^2 z_1^2), \quad (9)$$

$$B_0^A(\hat{\theta}) = -\frac{\phi_2}{2\phi_1^3} \left[ \left(1 + \frac{3}{2}\rho^2 z_1^2\right) z_{12} - \rho^2 z_1 z_2 \right], \quad (10)$$

where  $\rho, \phi_1, \phi_2$  denote the vectors modulus,  $z_1$  is the cosine of angle between  $\vec{\rho}$  and  $\vec{\phi}_1$ ,  $z_2$  – between  $\vec{\rho}$  and  $\vec{\phi}_2$ ,  $z_{12}$  – between  $\vec{\phi}_1$  and  $\vec{\phi}_2$ . The dispersion of  $\hat{\theta}$  is larger than for uncorrelated data because now it also accounts for the fluctuations due to systematic errors. As to the bias it remains zero for the linear model.

If systematic errors are multiplicative

$$y_i = (t_i + \mu_i \sigma_i)(1 + \lambda \eta_i), \quad (11)$$

where  $\eta_i$  quantify the systematic errors. If both statistical and systematic errors are small comparing with  $t_i$

$$y_i \approx t_i + \mu_i \sigma_i + \lambda \eta_i t_i,$$

the correlation matrix is

$$C_{ij} = \eta_i \eta_j t_i t_j + \delta_{ij} \sigma_i \sigma_j, \quad (12)$$

and the expressions for the bias and dispersion are the same as for the additive systematics case after the substitution  $s_i \rightarrow \eta_i t_i$ .

The Eqn. (9) can be split into the parts which correspond to the statistical and systematic fluctuations. One can see that when vectors  $\vec{\rho}$  and  $\vec{\phi}_1$  are orthogonal the systematic error on  $\hat{\theta}$  is equal to zero and the total dispersion is suppressed. Such suppression can be illustrated on the example of the extraction of asymmetry from the data with general offset error. Let  $f_i(\theta) = \theta x_i$  and both statistical and systematic errors are constant through the sample:  $s_i = s$ ,  $\sigma_i = \sigma$ . Then  $\rho_i = s/\sigma$ ,  $\phi_1^i = x_i/\sigma$  and  $z_1 \sim \sum x_i$ . If the positive and negative values of  $x_i$  compensate each other in the measurements,  $z_1 = 0$  and the systematic error vanishes. The appropriate data filtration can also be used to suppress the dispersion (9). To clarify the mechanism of this suppression let us trace the effect of a separate data point on the dispersion value. Add to the data set a point with statistical error  $\sigma_0$ , systematic error  $s_0$  and the data model  $f_0(\theta)$ . If the initial data set is large and the systematic error is comparable with statistics, i.e.

$$\begin{aligned} N &\gg 1, & \rho &\gg 1, \\ \phi_1 &\gg \frac{f'_0(\theta_0)}{\sigma_0}, & \rho \phi_1 z_1 &\gg \frac{s_0}{\sigma_0^2} f'_0(\theta_0), \end{aligned} \quad (13)$$

the change of  $D_0^A(\hat{\theta})$  after adding the new point is

$$\Delta D_0^A(\hat{\theta}) \approx \frac{2\rho}{\phi_1^3} \frac{1}{\sigma_0^2} \left[ z_1 s_0 f'_0(\theta_0) - \frac{\rho z_1^2}{\phi_1} [f'_0(\theta_0)]^2 \right]. \quad (14)$$

The second term in brackets is always negative and gives the decrease of dispersion due to improved statistical precision. At the same time the first term can be negative or positive, depending on the signs of  $z_1$  and  $s_0$ . Its absolute value can be larger than the absolute value of the second term and then  $D_0^A(\hat{\theta})$  can increase or decrease after adding the new point. This is manifestation of inconsistency of the SCE applied to the correlated data set. The balance between terms of Eqn. (14) is defined by the distribution of  $f'_i(\theta_0)/s_i$  and cuts of the tails of this distribution can decrease the estimator dispersion.

## 2 THE COVARIANCE MATRIX ESTIMATOR

If systematic error is additive and covariance matrix is known a priori and is given by (8) one can use for the parameter estimation the following functional minimization

$$\chi^2(\theta) = \sum_{i,j=1}^N (f_i(\theta) - y_i) E_{ij} (f_j(\theta) - y_j), \quad (15)$$

where  $E_{ij}$  is the inverted correlation matrix. This problem can be reduced to the uncorrelated case using the linear transformation of the vector  $\{f_i(\theta) - y_i\}$  and the estimator is linear for the linear data model. Besides, if statistical and systematics fluctuations obey the Gaussian distribution, this estimator provides minimal dispersion due to the Cramer-Rao inequality.

One can easily derive the expressions necessary to calculate the estimator bias and dispersion

$$\begin{aligned} \langle X \rangle &= 0, \\ \langle X^2 \rangle &= -a = \sum_{i,j=1}^N f'_i(\theta_0) E_{ij} f'_j(\theta_0), \\ \langle XY \rangle &= \frac{b}{3} = \sum_{i,j=1}^N f'_i(\theta_0) E_{ij} f''_j(\theta_0). \end{aligned}$$

Substituting in the above relations the explicit expression for  $E_{ij}$

$$E_{ij} = \frac{1}{\sigma_i \sigma_j} \left( \delta_{ij} - \frac{\rho_i \rho_j}{1 + \rho^2} \right)$$

we obtain the estimator dispersion

$$D_M^A(\hat{\theta}) = \frac{1}{\phi_1^2} \left[ 1 + \frac{\rho^2 z_1^2}{1 + \rho^2(1 - z_1^2)} \right] = \frac{1}{\phi_1^2} \xi_M, \quad (16)$$

where  $\xi_M$  is the ratio of the total dispersion to the pure statistical one. If  $\vec{\rho}$  and  $\vec{\phi}_1$  are collinear the dispersion of the estimator is

$$D_M^{A,\parallel}(\hat{\theta}) = \frac{1 + \rho^2}{\phi_1^2},$$

which coincide with the SCE dispersion (9). One can see that if  $\vec{\rho}$  and  $\vec{\phi}_1$  are not collinear the SCE dispersion (9) is always larger than the CME dispersion (16). This can be readily explained qualitatively. For SCE the fitted curve tightly follows the data points and, if these points are shifted due to the systematic errors fluctuations, the parameter gains appropriate systematic errors. At the same time, since for the CME the information on the data correlations is explicitly included in  $\chi^2$ , the correlated fluctuation of the data due to systematic shift does not necessary leads to the fitted curve shift and the parameter deviation gets smaller than for SCE. The exclusion occurs if  $z_1 = 0$ , when  $\vec{\rho}$  and  $\vec{\phi}_1$  are collinear and the systematic shift can be perfectly compensated by the change of parameter. If these vectors are orthogonal the CME dispersions is

$$D_M^{A,\perp}(\hat{\theta}) = \frac{1}{\phi_1^2}$$

i.e. it is just the same as the dispersion of SCE applied to the data set without correlations (6). Qualitatively it corresponds to the measurements scheme when systematic shift for the different points compensate each other, e.g. as in the example considered at the end of Sec. 1.

For the modern experiments systematic errors are often of the same order as statistical ones and if  $N \gg 1$  then  $\rho \gg 1$ . In this limit and if  $\vec{\rho}$  and  $\vec{\phi}_1$  are not collinear

$$D_M^A(\hat{\theta}) \approx \frac{1}{\phi_1^2(1 - z_1^2)} \quad (17)$$

and

$$D_0^A(\hat{\theta}) \approx \frac{\rho^2 z_1^2}{\phi_1^2}. \quad (18)$$

One can see that in the second case the estimator standard deviation rises linearly with the increase of the systematics, whereas the CME dispersion saturates. This difference can be illustrated on the numerical example inspired by the elastic proton-proton scattering. Let us choose

$$f_i = U \exp(-V x_i), \quad x_i = 0.1i,$$

where  $U = 100, V = 10, i = 1 \dots 9$ . Generating 100 data sets (7) with these  $f_i$  and

$$\sigma_i = 0.01 \sqrt{\frac{U}{f_i}}, \quad s_i = \frac{\kappa}{x_i} \quad (19)$$

we minimized functionals (2) and (15) varying  $U$  and  $V$  to obtain their estimators  $\hat{U}$  and  $\hat{V}$ . The values of  $(\hat{U} - U)^2$  and  $(\hat{V} - V)^2$  for all of the generated data sets were averaged to obtain the estimators dispersions. The results on the standard deviation of  $\hat{U}$  for different values of  $\kappa$  are given in Fig. 1 (the picture for  $\hat{V}$  is similar). One can see that at large  $\kappa$  the CME and the SCE standard deviations differ by factor of 3.

The example of dispersion suppression observed in the analysis of real experimental data can be found in Ref. [14]. In this paper we performed the leading order QCD fit to the inclusive deep inelastic scattering data of Refs. [15, 16] obtained by the BCDMS collaboration in order to determine the parton distribution functions and the strong coupling constant value  $\alpha_s$ . The two different estimators were used and the different estimates were obtained. For the SCE the standard deviation of  $\alpha_s(M_Z)$  is 0.015, while for the CME it is 0.007. The difference in the gluon distribution bounds for these estimators can be given in Fig. 2. One can see that the standard deviation of the gluon distribution for the CME is also about a half of the SCE standard deviation.

If  $z_1 \neq 1$ , the change of CME dispersion after adding a new point to the large sample as defined by Eqn. (13) is

$$\Delta D_M^A(\hat{\theta}) \approx -\frac{1}{\phi_1^4(1 - z_1^2)^2} \frac{1}{\sigma_0^2} \left[ f'_0(\theta_0) - \frac{\phi_1 z_1}{\rho} s_0 \right]^2.$$

This change is always negative that proves the CME consistency. Remind, that this is not necessary for the SCE (see Sec. 1). The same conclusion can be drawn from the comparison of Eqns. (17) and (18). Indeed, the CME dispersion falls with increase of statistical significance of the data set (i.e. decrease of  $\sigma$  or rise of  $N$ ) while the SCE dispersion does not. Note, that due to consistency of the CME the filtration procedure described in Sec. 1 is not meaningful for it.

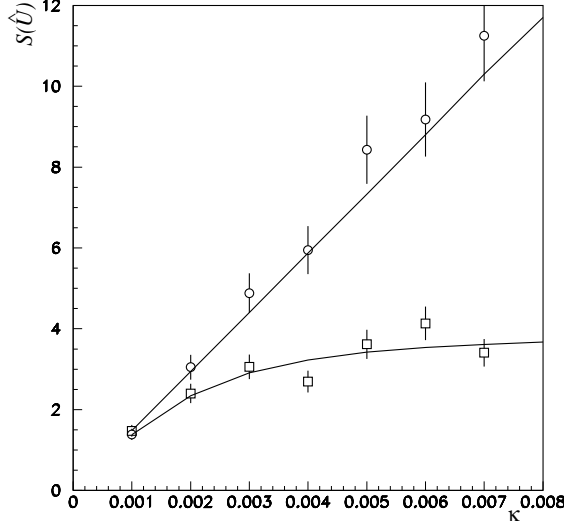


Figure 1: The standard deviations of SCE (circles) and CME (squares) for  $\hat{U}$  at different scales of systematic errors  $\kappa$ . The lines correspond to the calculation performed with the two-dimensional generalization of Eqns. (9,16).

The CME bias is

$$B_M^A(\hat{\theta}) = -\frac{\phi_1\phi_2}{2} \left[ D_M^A(\hat{\theta}) \right]^2 \left( z_{12} - \frac{\rho^2}{1+\rho^2} z_1 z_2 \right),$$

which vanishes for the linear data model and saturates in the limit of  $\rho \gg 1$  contrary to the SCE. In the numerical example (19) at  $\kappa = 0.007$  the CME bias is 0.07, whereas the SCE bias is 0.13.

For the multiplicative systematic errors the covariance matrix is unknown a priori and one is to calculate it using the parameter estimator. Proceeding this way in the minimization of the functional (15) we get

$$a = - \sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f'_j(\theta^0) - \frac{1}{2} \sum_{i,j=1}^N E''_{ij} C_{ij}. \quad (20)$$

The difference with corresponding expression for the case of additive systematic errors is in the second term of Eqn. (20). For the linear data model this term is

$$a^{(2)} = \frac{1}{2} \sum_{i,j=1}^N E''_{ij} C_{ij} = \frac{\phi_3^2}{2(1+\rho^2)^2} [\rho^4(z_3^2 - 1) - 3\rho^2 z_3^2 + 1],$$

where

$$\phi_3^i = \rho'_i = \frac{\rho_i}{f_i} f'_i(\theta^0) = \eta_i \phi_1^i,$$

$\phi_3$  is modulus of  $\vec{\phi}_3$  and  $z_3$  is the cosine of the angle between  $\vec{\phi}_3$  and  $\vec{\rho}$ . The ratio of the second term of Eqn. (20) to the first term  $a^{(1)} = \sum f'_i(\theta^0) E_{ij} f'_j(\theta^0)$  is

$$\frac{a^{(2)}}{a^{(1)}} = \frac{\phi_3^2}{\phi_1^2} \cdot \frac{\rho^4(z_3^2 - 1) - 3\rho^2 z_3^2 + 1}{(1+\rho^2)^2} \xi_M. \quad (21)$$



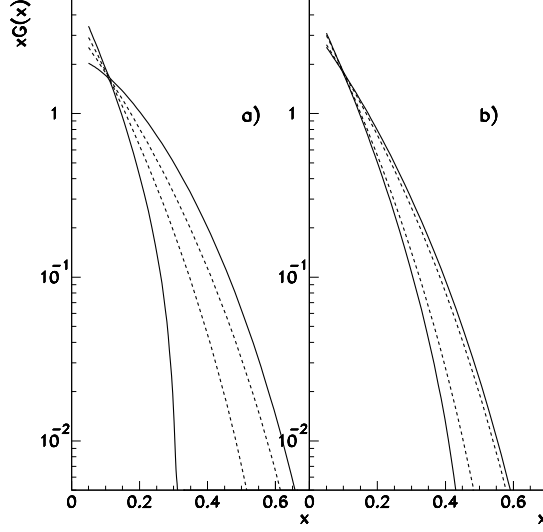


Figure 2: Bounds of gluon distribution obtained from the LO QCD fit to BCDMS data with different estimators (the SCE: a; the CME: b). Full lines correspond to the total experimental errors, dashed ones – to the statistical only.

If  $\xi_M \sim O(1)$  (that is valid for most real cases),  $a^{(2)} \sim O(\eta^2)a^{(1)}$  for all values of  $\rho$ , i.e. it is suppressed comparing with the first term for small  $\eta$ . Neglecting as elsewhere the third and fourth central moments of  $\{y_i\}$ , one can obtain that  $\langle X^2 \rangle \approx -a$  and the estimator dispersion for multiplicative systematic errors  $D_M^M \approx D_M^A$ .

In the case of multiplicative systematics errors Eqn. (3) is nonlinear even for the linear data model. As a consequence, the expressions responsible for the bias

$$\begin{aligned} \langle X \rangle &= \frac{1}{2} \sum_{i,j=1}^N E'_{ij} C_{ij}, \\ b &= 3 \sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f''_j(\theta^0) + 3 \sum_{i,j=1}^N f'_i(\theta^0) E'_{ij} f'_j(\theta^0) + \frac{1}{2} \sum_{i,j=1}^N E'''_{ij} C_{ij}, \\ \langle XY \rangle &= \sum_{i,j=1}^N f'_i(\theta^0) E_{ij} f''_j(\theta^0) + 2 \sum_{i,j=1}^N f'_i(\theta^0) E'_{ij} f'_j(\theta^0) - \frac{1}{4} \sum_{i,j=1}^N E''_{ij} C_{ij} \sum_{i,j=1}^N E'_{ij} C_{ij}, \end{aligned} \quad (22)$$

do not vanish even if  $f''_i(\theta)$  is equal to zero. Meanwhile the bias due to the estimator nonlinearity is small comparing with the estimator standard deviation. Since  $1/D_M^M \approx \langle X^2 \rangle \approx -a$  the bias of estimator with multiplicative systematic errors is

$$B_M^M(\hat{\theta}) \approx \sqrt{D_M^M(\hat{\theta})} \left[ \frac{\langle X \rangle}{\sqrt{-a}} + \frac{\langle XY \rangle - b/2}{(-a)^{3/2}} \right]. \quad (23)$$

The first term in the brackets of Eqn. (23) is

$$\frac{\langle X \rangle}{\sqrt{-a}} \approx -\frac{\phi_3}{\phi_1} \frac{\rho z_3}{1 + \rho^2} \sqrt{\xi_M} \sim O(\eta \sqrt{\xi_M}). \quad (24)$$

The contribution to the second term in brackets of Eqn. (23) from  $\sum f'_i(\theta^0)E'_{ij}f'_j(\theta^0)$  is proportional to

$$\frac{\phi_3}{\phi_1} \frac{\rho z_1}{(1+\rho^2)} \left( \frac{\rho^2}{1+\rho^2} z_1 z_3 - z_{13} \right) \xi_M^{3/2}$$

and hence it is  $\sim O(\eta \xi_M^{3/2})$ . As one can conclude from Eqns. (21,24) the contribution to the same term from  $\sum E''_{ij}C_{ij} \cdot \sum E'_{ij}C_{ij}$  is  $O(\eta^3 \xi_M^{3/2})$ . And finally since

$$\frac{1}{2} \sum_{i,j=1}^N E'''_{ij}C_{ij} = \frac{\rho z_1 \phi_3^3}{(1+\rho^3)^2} [\rho^4(z_3^2 - 1) + \rho^2(1 - 3z_3^2) + 2]$$

the contribution to Eqn. (23) coming from this term is  $O(\eta^3 \xi_M^{3/2})$ . In summary, for the linear data model the estimator bias is a sum of terms  $O(\eta^p \xi_M^q) D_M^M$  with  $p \geq 1$  and  $q \leq 3/2$ . Besides, at small  $\rho$  all the four contributions to the bias which survive for the linear data model are  $\sim \rho$  while at large  $\rho$  they are  $\sim 1/\rho$ . Summarizing, one can conclude that the estimator is negligible excluding the extreme cases with very large  $\xi_M$ .

The explicit estimate of the bias can be obtained from the Eqns. (22,23). Meanwhile it requires rather lengthy calculations and more simple tool for the bias evaluation is admirable. A convenient way for this is to trace the net residual

$$R = -\frac{1}{N} \sum_{i=1}^N \frac{f_i(\hat{\theta}) - y_i}{\sqrt{\sigma_i^2 + s_i^2}}.$$

Expanding  $f_i(\theta)$  near  $\theta_0$  and keeping only the first term in Eqn. (4) one obtains for the sample (7)

$$R \approx -\frac{1}{N} \sum_{i=1}^N \frac{\mu_i + \lambda \rho_i}{\sqrt{1 + \rho_i^2}} + (\hat{\theta} - \theta_0) \frac{1}{N} \sum_{i=1}^N \frac{\phi_1^i}{\sqrt{1 + \rho_i^2}}.$$

If the estimator is unbiased, the value of  $R$  averaged over the samples is equal to zero. Nevertheless the particular values of  $R$  may be not equal to zero due to fluctuations. For the limited  $\xi_M$  the dispersion of  $R$  is

$$D(R) = \frac{1}{N^2} \sum_{i,j=1}^N \frac{\delta_{ij} + \rho_i \rho_j}{\sqrt{1 + \rho_i^2} \sqrt{1 + \rho_j^2}} + O(1/N). \quad (25)$$

If the analyzed data come from a single experiment with dominating systematics (i.e with  $\rho > 1$ ) then  $D(R) \sim 1$ . In particular for the BCDMS data of Refs. [15, 16]  $D(R) \approx 0.7$ . For  $N_{exp}$  independent experiments involved in the analysis  $D(R) \sim 1/N_{exp}$ . Comparing the net residual  $R$  with this value allows to get a guess about the estimator bias. More definite conclusion can be drawn after the comparison of  $R$  with its dispersion calculated using Eqn. (25).

### 3 PLANNING OF THE COUNTING EXPERIMENTS

In a particular case when the differential cross section on the variable  $x$  is measured, the predicted average number of events in the  $i$ -th bin of is

$$\langle N_i \rangle = L f_i \Delta x_i \beta_i,$$

where  $L$  is the integral experiment luminosity,  $\beta_i$  is the registration efficiency, and  $\Delta x_i$  is the bin width. Neglecting the fluctuations of  $N_i$  the statistical error on the  $i$ -th measurement is

$$\sigma_i = \frac{\sqrt{\langle N_i \rangle}}{L \Delta x_i \beta_i}$$

and

$$\frac{1}{\sigma_i^2} = \frac{L \beta_i}{f_i} \Delta x_i.$$

The scalar product of the vectors  $\vec{\rho}$  and  $\vec{\phi}$  is

$$(\vec{\rho} \cdot \vec{\phi}) = L \sum_{i=1}^N \frac{f'_i s_i}{f_i} \beta_i \Delta x_i$$

and

$$\phi^2 = L \sum_{i=1}^N \frac{[f'_i]^2}{f_i} \beta_i \Delta x_i, \quad \rho^2 = L \sum_{i=1}^N \frac{[s_i]^2}{f_i} \beta_i \Delta x_i.$$

For the dense measurements these scalars can be reduced to the integrals over the measurements region  $\Omega$ :

$$(\vec{\rho} \cdot \vec{\phi}) = L \int_{\Omega} f'(x) s(x) d\tilde{x}$$

and

$$\phi^2 = L \int_{\Omega} [f'(x)]^2 d\tilde{x}, \quad \rho^2 = L \int_{\Omega} [s(x)]^2 d\tilde{x},$$

where  $d\tilde{x} = \beta(x)/f(x)dx$ . The latter expressions can be used in the equations for the estimators dispersions<sup>3</sup>. This approach is convenient for the future experiment optimization since it allows for to analyze integrated expression in order to search for the optimal region of measurements. For the simple functions  $f(x)$ ,  $\beta(x)$ , and  $s(x)$  such analysis sure can be performed analytically.

## 4 CONCLUSION

In conclusion, the CME is a convenient tool for the analysis of the data sets with the account of correlations due to systematic errors. The CME is consistent for the realistic cases (when systematic errors on the fitted parameters are not extremely large comparing with the statistical ones) and its dispersion is always smaller, than the dispersion of the  $\chi^2$  estimator without account of correlations. The estimator bias is negligible for the realistic cases if the covariance matrix is calculated during the fit iteratively using the parameter estimator itself. Analytical formula for the covariance matrix inversion allows to perform fast and precise calculations even for very large data sets. The latter is especially important in view of numerical instabilities occurring in the fits to precise data in the case of large correlation between the fitted parameters (see in this connection Ref. [17]).

A particular attention should be paid on the connection between the estimator dispersion and the confidence interval. For a known distribution of the estimator the confidence interval can be easily calculated (e.g. it is well known that for the Gaussian distribution one standard

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<sup>3</sup>As a result one obtains the Fisher's information for the correlated data case.

deviation corresponds to the 67% confidence level). Unfortunately due to the possible non-Gaussian nature of the systematic errors one cannot prove that an estimator accounting for systematics is Gaussian distributed. However for the large number of systematic errors of comparable scale the estimator should obey Gaussian distribution just to the central limit theorem of statistics. Otherwise the robust estimates of the confidence intervals, e.g. Chebyshev's inequality, should be used.

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